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DATE: April 4, 1974

To : File

FROM : Joshua Lederberg

SUBJECT: Meeting with Al Feldman of the Walter Reed Institute for Medical Research

Feldman is in charge of a substantial file of chemicals being tested as drugs for malaria and other infections and is particularly interested in the area of structure activity correlation. These structures have been coded in a way that Feldman believes gives unambiguous structural information. However, he is concerned that their formats are incompatible with those of the NCI or of Chemical Abstracts. After some discussion, however, it appeared to us that it would not be difficult to transform all of those formats to some conventional connection tables, so that an interface should be possible. There are all the usual problems of identifying chronological forms or tautomerisms. Feldman agreed to send us some examples of his formats, and we agreed to take a look at the problem that would be entailed in translating them to a standardized connection table.

It is not entirely clear what use would be made of all this. We indicated that our own research interest in this particular area was somewhat limited but that we would be glad to facilitate others who wish to concentrate in this particular vein. We would be able to offer the SUMEX facilities, the DENDRAL tools and some time in providing backup. However, it is possible that other groups like Wipke will want to take a more aggressive role than we do.

Feldman also mentioned that there are contrasting efforts at the National Cancer Institute, and that we might do well to make contact with Barbara Murray with respect to their cancer chemotherapy file. He commented that Chemical Abstracts would be less useful except for bibliographic purposes since the only content information attached to the structures would be the index pointers to Chemical Abstracts itself. We did not bring up the question of how prophet would relate to all of this.

All in all it is not really clear what can or ought to be done but we at least ought to try to stay in touch with the situation to see if we cannot catalyze a somewhat more unified approach to structure handling now that a network is eminent. This is not the primary mandate of SUMEX itself but does come somewhat closer to DENDRAL.

I will ask Elliott to oversee this whole matter.

P.S. The recent American Chemical Society Abstracts were cited as having a large number of references to people working in chemical information processing.